



EMSP

Environmental Management Science Program

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ANALYTICAL CHEMISTRY AND INSTRUMENTATION

FUNDAMENTAL STUDIES OF IMPROVED METHODS FOR DETERMINATIONS OF THE MOST COMMON CONTAMINANTS AT DOE SITES CAN CONTRIBUTE TO IMPROVED RELIABILITY AND REDUCED COSTS

Perhaps nothing is so commonplace in the Department of Energy (DOE) complex as the analytical laboratories that play a major role in detecting contaminants and monitoring their remediation. Hence, fundamental studies of analytical procedures and methods in those areas most common at DOE sites can significantly reduce environmental restoration costs.

Sensitive and selective detection of dense nonaqueous phase liquids (DNAPLs) and other organic compounds in the subsurface is important at almost all DOE sites. One EMSP project is directed toward a fundamental understanding of new methods to enhance detector sensitivity for organic compounds by increasing their tendency to form negative ions.

Determining the amount of heavy metals in samples is also a common procedure for DOE facilities. One EMSP project is developing a system to measure the elemental composition of samples directly (without laboratory preparations) using laser-induced breakdown spectroscopy. Another project is developing inexpensive electrochemical sensors for in-situ monitoring of trace quantities of uranium and chromium.

As certain microbes can degrade organic pollutants, microbial bioremediation is an attractive cleanup strategy. Thus, an ability to monitor the genes in soil samples that code for enzymes capable of degrading specific pollutants is important in assessing bioremediation treatment. One EMSP project is evaluating a monitoring strategy for a naphthalene-degrading gene by the use of a DNA diagnostic procedure with mass spectrometry. Another project is developing a rapid screening assay for a bacterial enzyme that can oxidize trichloroethylene, a common DNAPL contaminant.

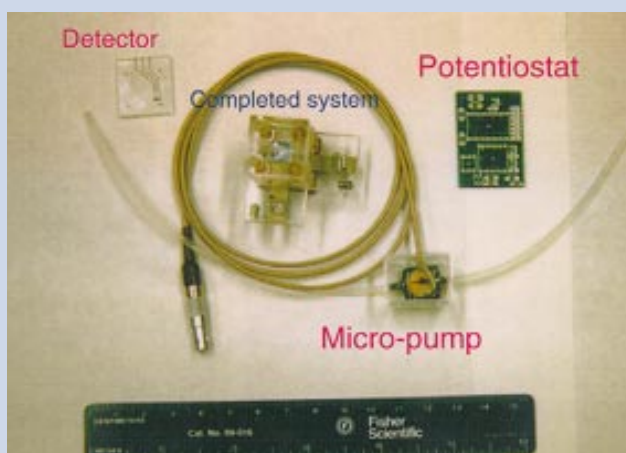
The Argonne National Laboratory Advanced Photon Source has a unique capability to produce intense x-rays for x-ray absorption studies. One EMSP project will build a beamline that will allow Environmental Management scientists to use this facility.

PROBLEMS/SOLUTIONS

- The most sensitive methods for detection of highly-chlorinated organic compounds rely on the formation of negative ions, but most organic compounds are detected by less sensitive techniques because they do not readily form negative ions. Studies of recently discovered methods to enhance the formation of negative ions may lead to improved, inexpensive detectors for routine analyses.
- Laboratory determinations of heavy metal contaminants are common in the DOE complex, but on-site determinations would often be more appropriate and less expensive. A study of laser-induced breakdown spectroscopy may assist development of more reliable field measurements using that technique, and new electrochemical devices are being studied for deployment as continuous, in-situ monitors for uranium and chromium at parts per billion levels in water.
- Current laboratory-based methods for monitoring microbes are cumbersome and expensive. Two EMSP projects are developing new procedures for rapid, less expensive assays.
- The Advanced Photon Source will provide a unique source of intense x-rays for fundamental research in many areas related to studies of materials. One EMSP project is developing a beamline to make this resource available to the Environmental Management community.

ANTICIPATED IMPACT

- Site Technology Coordinating Group needs for improved techniques for monitoring Resource Conservation and Recovery Act metals are cited at Idaho, Savannah River, and Hanford, for example. Eight sites described needs for improved DNAPL characterization.
- Among the highest priority needs cited in the Hanford Subsurface Contaminant Science Needs is that for improved monitoring instruments for carbon tetrachloride, trichloroethylene, chromium, and uranium. Each of these areas is the subject of at least one EMSP project.
- Real-time chemical groundwater monitoring techniques are needed to cut analysis costs where post-remediation monitoring of aquifers may be required for many years.



New Methods for Elemental Analysis

The electrochemical metal microanalyzer, shown here, is designed to detect uranium and chromium at parts per billion concentrations. The pocket-sized microanalyzer is being developed by New Mexico State University and Pacific Northwest National Laboratory.

Detection of Organic Compounds

The University of Tennessee/Oak Ridge National Laboratory team has been investigating methods to develop novel analytical techniques for the inexpensive detection of a wide variety of organic molecules with high sensitivity. Electron capture with the resulting formation of negative ions is widely used in sensitive but inexpensive detectors for highly-chlorinated organics, but this technique does not work with most organic species. It has recently been discovered that electron attachment and the subsequent formation of negative ions is enhanced by up to a hundred thousand times if the molecule is in a highly-excited state. Molecules can be produced in these highly-excited states by laser excitation or in a glow discharge. Efficient formation of negative ions in benzene and toluene was observed, and it was found that weak electric and magnetic fields further enhance ion formation.

New Methods for Elemental Analysis

Many people have heated an object by using a simple lens to focus sunlight on it. When a laser pulse is focused on a surface, a small amount of the surface can be vaporized with sufficient energy to cause ionization of the vapor with resulting light emission that is characteristic of the species that were vaporized. The University of South Carolina group is conducting a fundamental study of laser-induced breakdown spectroscopy (LIBS) using fiber optics for remote measurements of trace metals. One objective has been to determine factors that affect selective vaporization, which is a serious problem for making reliable quantitative measurements. In addition, this group has performed the first demonstration of LIBS imaging using fiber optics, and they have combined LIBS and Raman spectral imaging in a single probe. Thus, the spatial distribution of both elemental and molecular species can be determined with the same apparatus.

A major goal of the New Mexico State University/Pacific Northwest National Laboratory project has been the development of a miniaturized electrochemical sensor for uranium and chromium at parts per billion (ppb) concentrations. The pocket-sized microanalyzer includes a stack of modules to perform selective chemical reactions followed by an electrochemical detector. A submersible probe for these two metals has also been studied, and the goal of this work is to produce an inexpensive probe that can be left in a well, for example, to monitor metal concentrations at ppb levels without expensive sampling and laboratory analyses. This probe incorporates a microdialysis sampling procedure that may enable in-situ sensing of metal speciation.

Diagnostics for Bioremediation

The Lawrence Berkeley National Laboratory group has investigated methods to use DNA-based procedures for the detection of a naphthalene-degrading gene. They have used a peptide nucleic acid probe to identify a polymerase chain reaction (PCR) product from a naphthalene-degrading organism. Matrix-assisted-laser-desorption-ionization time-of-flight mass spectrometry (MALDI-TOF-MS) was found to offer the possibility for automation with rapid detection, as is needed to track the course of bioremediation over large, polluted areas.

In another demonstration of the feasibility of MALDI-MS detection of bacterial PCR products, the Oak Ridge National Laboratory/University of Washington team has developed an assay for a certain gene in two species of bacteria that metabolize trichloroethylene. They have also found that MALDI-TOF-MS detection of PCR-amplified bacterial targets offers promise as a rapid method for assessing the potential of microbial populations for bioremediation. These new methods could replace current laboratory-based methods that are cumbersome and expensive.

The Pacific Northwest Consortium and coworkers team is building a beamline to access the Advanced Photon Source at Argonne National Laboratory. This facility will make an intense x-ray source available for various forms of x-ray absorption spectroscopy for basic research on topics such as chemical speciation of tank wastes, radiation-induced structural changes in waste forms, verification of modeling for transport of contaminants under geologic conditions, and many other potential uses by the Environmental Management community.

PROJECT TEAMS

(EMSP AWARD NUMBER)

- New Mexico State University
Pacific Northwest National Laboratory
(54639)
- Lawrence Berkeley National Laboratory
(54698)
- Pacific Northwest Consortium –
Collaborative Access Team
University of Washington
Pacific Northwest National Laboratory
Simon Fraser University
(54800)
- Oak Ridge National Laboratory
University of Washington
(55108)
- University of South Carolina (55205)
- University of Tennessee
Oak Ridge National Laboratory
(55328)



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